A Dynamical Decomposition of the Hamiltonian for Analyzing the Time Evolution of Quantum Mechanically Driven Harmonic Oscillator Systems

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For analyzing the time evolution of quantum mechanically driven harmonic oscillator systems, we first establish the eigenvalue equation for the time-evolved wave function, and then we dynamically decompose the Hamiltonian into two parts. One part is the operator which does not change the state, and the other part does. Through this decomposition, the time evolution of the state can be solved more easily than in the familiar way. We illustrate this method by exactly solving the system of the driven harmonic oscillator. We show that nonspreading wave packets can also exist in this system in addition to the historically known paradigms, the profiles of which are the same as those in the harmonic oscillator system.

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I. INTRODUCTION

In 1926, Schrödinger constructed the first nonspreading wave packet (NSWP) with the profile of the ground state of a simple harmonic oscillator (SHO) \cite{1}. This example shows that a NSWP exists in a system with the Hamiltonian $H(t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$. In 1954 Senitzky generalized Schrödinger’s result, constructing NSWPs with the profiles of high energy eigenstates of a SHO \cite{2}. Other type of NSWPs were found in 1979 by Berry and Balazs \cite{3}. They showed that NSWPs exist in a system with Hamiltonian $H(t) = \frac{p^2}{2m}$, that is free space, and also in a system with the Hamiltonian $H(t) = \frac{p^2}{2m} - F(t)x$, with the solution of an Airy wave packet. Lin et al. derived the general potential $V(x,t)$ that the Airy wave packet will remain nonspreading \cite{4}. Besides these theoretical works, NSWPs attracted intensive experimental investigations. Some recent optical observations of NSWPs can be found in Refs. \cite{6–8}. Comparing the Hamiltonian of these two types of NSWPs, we may suspect that NSWPs should also exist in a system with $H(t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 - F(t)x$, which is the driven or forced harmonic oscillator. Also we expect that the profiles will not be altered from those in the SHO. We proposed in this paper the method of dynamical decomposition for solving the time-dependent Schrödinger equation (TDSE). As an application, we analytically and numerically elucidate that wave packets in the driven SHO can be nonspreading, and are indeed with the same profiles as those in the SHO.

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It is the Hamiltonian that governs the change in time of the wave function $\Psi(x,t)$. And the time evolution of system is described by the TDSE

$$i\hbar\partial_t\Psi(x,t) = H(t)\Psi(x,t).$$

We discuss the general case in which the Hamiltonian is time dependent. The Schrödinger equation shows that the action of the Hamiltonian $H(t)$ on the wave function $\Psi(x,t)$ gives the rate change in time of $\Psi(x,t)$. In principle, integrating all these infinitesimal changes shows how the wave function evolves from an initial state $\Psi(x,t=0)$ to $\Psi(x,t)$. However, the result of the action of $H(t)$ on $\Psi(x,t)$ in general is complicated. And hence analytical solutions of Eq. (1) are difficult to obtain and are rare. For some cases, such as systems like the simple harmonic oscillator or free space, the exact solutions may be obtained by the Green’s function or propagator methods. For a recent work using this method to obtain exact solutions one may refer to Dijk et al. [9]. For an early reference, one may be referred to Barone et al. [10], which shows different methods for obtaining the propagator. For a time-periodic Hamiltonian, Floquet theory is powerful and the numerical exact solution can be obtained. For a related review article, one can refer to Chu [11].

To analyze the TDSE generally, we decompose the Hamiltonian $H(t)$ into

$$H(t) = H_0 + H_{int}(t),$$

Where $H_0$ is time independent and $H_{int}(t)$ is time dependent. We then expand the wave function in terms of eigenstates of the Hamiltonian $H_0$ [12–14]. That is

$$\Psi(x,0) = \sum_n c_n \phi_n(x), \text{ and}$$

$$\Psi(x,t) = \sum_n c_n(t) \phi_n(x).$$

The time evolution of $\Psi(x,t)$ is expressed in terms of the time dependent coefficients $c_n(t)$, which should be determined by substituting Eq. (4) to Eq. (1). We then have to solve a system of coupled equations. In this paper, we develop another method for analyzing the time evolution of the TDSE. We follow the spirit of Eq. (2) decomposing the Hamiltonian into two terms. Our motivation is that it would be helpful at each instant to know those operators which do not change the time-evolved state. The Hamiltonian can then be decomposed dynamically according to these operators into two parts. One part is the state-preserving operator which does not change the state. The other part is the state-changing operator which changes the state. By a proper choice of state-preserving operator, the state-changing operator may be reduced to a simpler form, and then the time evolution of a wave function can be solved more easily. We introduce this method in the following.

The situation that an operator does not change a state corresponds to an eigenvalue equation. To find eigenvalue equations for a time-evolving state $\Psi(x,t)$ would seem difficult as we have not yet solved the Schrödinger equation. However, there is a way to find eigenvalue equations of $\Psi(x,t)$. Consider a wave function evolving from an initial wave $\Psi(x,t=0)$. We then have the following relation

$$\Psi(x,t) = U(t,0)\Psi(x,0),$$
where \( U(t,0) \) is the time evolution operator. \( U(t,0) \) is unitary with Hermitian Hamiltonian \( H(t) \). By means of the time evolution operator, we can carry out a unitary transformation of states, operators, and also eigenvalue equations. At time \( t = 0 \), let the initial eigenvalue equation for \( \Psi(x, t=0) \) be

\[
\tilde{H}(0)\Psi(x,0) = \tilde{E}(0)\Psi(x,0),
\]

where \( \tilde{H}(0) \) is some operator defined at time \( t=0 \), which may represent a position operator, a momentum operator, an energy operator, etc., and \( \tilde{E}(0) \) is the corresponding eigenvalue. Operating \( U(t,0) \) on both sides of Eq. (6) yields the eigenvalue equation at time \( t \)

\[
\tilde{H}(t)\Psi(x,t) = \tilde{E}(t)\Psi(x,t),
\]

\[
\tilde{E}(t) = \tilde{E}(0),
\]

where \( \Psi(x, t=0) \) is transformed to \( \Psi(x, t) \), and \( \tilde{H}(0) \) is transformed to \( \tilde{H}(t) \) which is defined by

\[
\tilde{H}(t) = U(t,0)\tilde{H}(0)U^{-1}(t,0).
\]

Eq. (7) is the eigenvalue equation of \( \Psi(x, t) \). And \( \tilde{H}(t) \) is the state-preserving operator we are looking for. Let \( H_c(t) = H(t) - \tilde{H}(t) \). Then \( H_c(t) \) is the state-changing operator. The Hamiltonian is thus decomposed into

\[
H(t) = \tilde{H}(t) + H_c(t).
\]

We call Eq. (10) the **dynamical decomposition**, as \( \tilde{H}(t) \) is adjusted according to the time evolution of the wave function. From Eq. (10), the Schrödinger equation can be written in a simpler form as

\[
\frac{i\hbar}{\hbar}\partial_t\Psi(x,t) = H(t)\Psi(x,t) = [\tilde{E}(t) + H_c(t)]\Psi(x,t).
\]

Eq. (11) is the formula we use to solve \( \Psi(x,t) \). The decomposition of the Hamiltonian is particularly interesting when the only effect of \( H_c(t) \) is to result in a spatial shift of the packet. This corresponds to the case of nonspreading wave packets (NSWPs). In the following, we apply the method of dynamical decomposition to study the time-dependent driven SHO.

**II. EVOLUTION OF THE WAVE FUNCTION \( \Phi_n(x) \) IN DRIVEN SIMPLE HARMONIC OSCILLATOR**

We discuss the time evolution of the driven harmonic oscillator. The Hamiltonian is defined below:

\[
H(t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 - F(t)x,
\]
where $F(t)$ is an arbitrary function of time. We consider the initial eigenvalue equation at time $t = 0$ as
\[
(p^2/2m + \frac{1}{2}m\omega^2x^2)\Phi_n(x) = E_n\Phi_n(x),
\]
where $\Phi_n(x)$ is the $n$-th eigenfunction of the SHO, with eigenvalue $E_n = (n + 1/2)\hbar\omega$, $n = 0, 1, 2, \cdots$. That is, we start from
\[
\Psi(x, 0) = \Phi_n(x),
\]
\[
\tilde{H}(0) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2.
\]
This choice of initial state does not lose generality, as any initial state can be composed from the set of $\Phi_n(x)$. From Eq. (9) and Eq. (15), we have
\[
\tilde{H}(t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 t,
\]
where
\[
x_t = U(t, 0)xU^{-1}(t, 0),
\]
\[
p_t = U(t, 0)pU^{-1}(t, 0).
\]

The Hamiltonian is time-dependent, the calculation of $x_t$ and $p_t$ can be done by the following procedure. For instance, to calculate $x_t$, we begin with setting, $x_t = A(t)x + B(t)p + C(t)$, then
\[
x_{t+dt} = U(t + dt, t)x_tU^{-1}(t + dt, t)
= \exp[-i\hbar H(t)dt]x_t \exp[i\hbar H(t)dt]
= x_t - \frac{i}{\hbar}dt[H(t), x_t]
= A(t + dt)x + B(t + dt)p + C(t + dt).
\]
Applying the boundary condition that $A(0) = 1, B(0) = 0, C(0) = 0$, we can determine $A(t), B(t), C(t)$, and therefore $x_t$. Going through this calculation then yields
\[
x_t = \cos(\omega t)x - \frac{\sin(\omega t)}{m\omega}p + \frac{1}{m\omega}f_s(t),
\]
\[
p_t = m\omega \sin(\omega t) + \cos(\omega t)p - f_c(t),
\]
where
\[
f_s(t) = \int_0^t F(\tau) \sin \omega \tau d\tau,
\]
\[
f_c(t) = \int_0^t F(\tau) \cos \omega \tau d\tau.
\]
Substituting Eqs. (20) and (21) into (16), we obtain the following results:

\[
\tilde{H}(t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - \dot{d}(t)p + (m\ddot{d}(t) - F(t))x \\
+ \frac{1}{2m}[f_s(t)^2 + f_c(t)^2], \quad \text{(24)}
\]

\[
\tilde{E}(t) = E_n, \quad \text{(25)}
\]

\[
H_c(t) = H(t) - \tilde{H}(t) \\
= \ddot{d}(t)p - m\dddot{d}(t)x - \frac{1}{2m}[f_s(t)^2 + f_c(t)^2], \quad \text{(26)}
\]

where

\[
d(t) = \frac{1}{m\omega} \int_0^\infty F(\tau) \sin(\omega(t - \tau)) d\tau. \quad \text{(27)}
\]

\(H_c(t)\) in Eq. (26) is linear in \(x\) and \(p\), this is in fact an indication of NSWP [5]. From Eqs. (11), (25), and (26), the Schrödinger equation is an equation linear in \(x\) and \(p\), we can easily solve it and obtain the result as follows:

\[
\Psi(x, t = 0) = \Phi_n(x), \\
\Psi(x, t) = \exp\left[\frac{i}{\hbar}(\theta(x, t) + m\ddot{d}(t)x)\right]\Phi_n(x - d(t)), \quad \text{(28)}
\]

where

\[
\theta(x, t) = -E_n t + \int_0^t \left[\frac{1}{2m}(f_s(\tau)^2 + f_c(\tau)^2) + m\ddot{d}(\tau)^2\right] d\tau. \quad \text{(29)}
\]

Our result can be compared to a known solution [15]. However, we obtain the exact solution for broader initial conditions, and particularly we show the existence of NSWP in this system. Eq. (28) shows that \(\Psi(x, t)\) is an NSWP, with \(\phi_n(x)\) as the profile and its motion is described by the trajectory: \(x = d(t)\). It is interesting to note that \(d(t)\) in fact is the solution of the equation

\[
\ddot{d} + \omega^2 d(t) = F(t)/m, \quad \text{(30)}
\]

which is just the classical equation of the driven harmonic oscillator, defined in Eq. (12). This shows that this NSWP propagates just like a classical particle whose motion obeys the classical dynamics of the Hamiltonian \(H(t)\). We thus get the illustrative result that the driven simple harmonic system does allow the existence of NSWP, no matter how complicated the driving force \(F(t)\) is. It seems that this result has not been discussed before to our knowledge.

Taking \(n = 0\) in Eq. (28), then \(\Psi(x, t)\) is proportional to \(\Phi_0(x - d(t))\), which represents a displaced ground state, and is known as a coherent state. This leads to the well-known result that the probability distribution among states is a Poisson distribution.
III. NUMERICAL SIMULATIONS

For an illustration of the developed Hamiltonian decomposition method, we consider a ground state electron moving in a harmonic potential and being excited by a sine-squared laser pulse with carrier frequency $\Omega$. That is

$$F(t) = F_m \sin^2\left(\frac{\pi t}{T}\right) \sin(\Omega t) \text{ for } 0 \leq t \leq T, = 0 \text{ otherwise.}$$

The corresponding $d(t)$ in Eq. (27) can be derived explicitly. For a nonresonant excitation ($\Omega \neq \omega$) and $0 \leq t \leq T$, we have (with $\Lambda \equiv \frac{2\pi}{T}$)

$$d(t) = \frac{F_m}{2m\omega(\omega^2-\Omega^2)} \left[ \frac{\omega \sin \Omega t - \Omega \sin \omega t}{\omega^2-(\Lambda-\Omega)^2} - \frac{\omega \sin[\Lambda t - \Omega t]}{\omega^2 - (\Lambda - \Omega)^2} + \frac{\omega \sin[\Lambda t + \Omega t]}{\omega^2 - (\Lambda + \Omega)^2} \right].$$

For a resonant excitation ($\Omega = \omega$),

$$d(t) = \frac{F_m}{4m\omega} \left\{ \frac{\sin \omega t}{\omega} - t \cos \omega t - \frac{2\omega \sin \omega t}{4\omega^2 - \Lambda^2} - \frac{\omega \sin[\omega t - \Lambda t]}{\Lambda(2\omega - \Lambda)} \right\}.$$

We discretize the system by the Fourier-Grid-Hamiltonian method [16, 17]. Jiang [18] has applied the method to study the high-frequency stabilization of an excited Morse oscillator under intense fields. We integrate the time-dependent Schrödinger equation by the variable-step Adams method [19]. During the excitation, we calculate the energy expectation of the oscillator by

$$\langle H(t) \rangle = \langle \frac{p^2}{2m} \rangle + \frac{1}{2} \omega x^2(t) - F(t)x(t).$$

And the acceleration function through Ehrenfest’s theorem:

$$m\langle \ddot{x}(t) \rangle = -\langle \frac{\partial H}{\partial x} \rangle = F(t) - m\omega^2 x(t).$$

Also we calculated the uncertainty $\Delta x, \Delta p$ and the product $\Delta x \cdot \Delta p$ during the excitation duration. We perform the calculation of the nonresonant ($\Omega = \omega/2$) and resonant ($\Omega = \omega$) excitations with $F_m = 1, T = 10 - \text{cycle (cycle = } 2\pi/\Omega)$. In Fig. 1(a), we show the peak of the wavepacket versus time and the classical analytic $d(t)$ of the nonresonant excitation. The peaks (blue-dots) are coincident with $d(t)$ (red-line) and both are in phase with the field $F(t)$ (gray-dashed). Fig. 1(b) are the corresponding results of resonant excitation. The wave peaks (blue-dots) are also coincident with the classical $d(t)$ in our theory. From Eq. (33), $t \cos \omega t$ is dominant at larger $t$, as depicted.
FIG. 1: Fig. 1(a): The calculated wave peak position in time (blue-dots) and trajectory of a driven classical oscillator $d(t)$ (red-line) of a typical nonresonant excitation with pulse $F(t)$ (gray-dashed, label in the left axis). The parameters are described in context. Fig. 1(b): The corresponding results of a resonant excitation. Near the tail of the pulse, the field is vanishing but the wave peak position oscillates at $\sim t \cos \omega t$ as predicted.

FIG. 2: Fig. 2(a): The expectation value of time dependent Hamiltonian $\langle H(t) \rangle$ and the Ehrenfest acceleration function for the nonresonant case. Fig. 2(b): The corresponding results of the resonant case. Near the vanishing pulse tail, the wave packet is still accelerating. The wavepacket peaks are not in phase with field $F(t)$ (gray-dashed) in the resonant case. Fig. 2(a) shows the expectations of the energy $\langle H(t) \rangle$ (red-line) and acceleration $\ddot{d}$ (blue-dots) of the nonresonant case. $\langle H(t) \rangle$ starts from the energy (0.5 au) of the ground state, absorbs photons from the field, oscillates with the field and returns to 0.5 at the vanishing of field. The acceleration shows similar oscillating with the field. Fig. 2(b) are the corresponding results of the resonant case. $\langle H(t) \rangle$ (red-line) and $\ddot{d}$ (blue-dots) are increasing with time to quite large values in the resonant excitation. Finally in Fig. 3 we depict the time behaviors of the uncertainty $\Delta x, \Delta p$ and the product $\Delta x \cdot \Delta p$ of the resonant case. The minimum uncertainty (coherent state) was shown through the excitation. As shown in Figs. 1(b) and 2(b), the energy $\langle H(t) \rangle$ goes to much larger values than the initial (0.5), and the wave peaks $d(t)$ run far beyond the classical turning points ($x \pm 1$) in the resonant excitation. However, the constant uncertainty holds throughout the pulse duration and the shape of the wavepacket remains unchanged. The same results are obtained for the nonresonant case.
IV. CONCLUSIONS

We have shown the dynamical decomposition method for analyzing the time evolution of a quantum mechanical system. The eigenvalue equation of the wave function at each instant is used. The eigenvalue equation in general includes the operator $p^2/2m$, hence the state-changing operator $H_c(t)$ is simpler. We exactly solve the driven harmonic oscillator, we also show that this system allows the existence of NSWPs. This is due to the state-changing operator $H_c(t)$ being linear in $x$ and $p$, as shown by Lin [5]. It is interesting to note that in a Hamiltonian system, if it allows the existence of NSWPs, then it seems that adding a driving term $F(t) \cdot x$ to the Hamiltonian will neither destroy the existence nor change the profile of the NSWPs. We justify our theoretical results by numerical simulations. The peak position of the wave packet follows the trajectory of a classical driven oscillator. And the nonspreading property of the wavepacket remains under both resonant and nonresonant excitations. This decomposition method can be applied to analyze the time evolution of general Hamiltonian systems as well. Further applications are under investigation.
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References